



chain nodes :

13 20 21 23 25 27 34 37 38 45 46 47 48

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 14 15 16 17 18 19 28 29 30 31 32 33 39 40
41 42 43 44 49 50 51 52 53 54

chain bonds :

2-27 12-13 13-16 19-25 20-21 20-23 20-38 20-48 21-37 25-45 27-46 33-34 34-47 38-42
48-54

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 14-15 14-19 15-16 16-17
17-18 18-19 28-29 28-33 29-30 30-31 31-32 32-33 39-40 39-44 40-41 41-42 42-43
43-44 49-50 49-54 50-51 51-52 52-53 53-54

exact/norm bonds :

2-27 19-25 20-23 21-37 33-34 38-42 48-54

exact bonds :

12-13 13-16 20-21 20-38 20-48 25-45 27-46 34-47

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 14-15 14-19 15-16 16-17
17-18 18-19 28-29 28-33 29-30 30-31 31-32 32-33 39-40 39-44 40-41 41-42 42-43
43-44 49-50 49-54 50-51 51-52 52-53 53-54

G1:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu

G2:[*1],[*2],[*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS
23:CLASS 25:CLASS 27:CLASS 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS
37:CLASS 38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:CLASS 46:CLASS
47:CLASS 48:CLASS 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom

